

beta-Alanine, N-methyl-
2679-14-3 | DTXSID10181298

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.26 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.20e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

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beta-Alanine, N-methyl-

Measured: 8.82e-01

Predicted: 1.26

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Proline

Measured: 1.41

Predicted: 1.47

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N-Methylolacrylamide

Measured: 6.46

Predicted: 4.91

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N-Methylglycine

Measured: 3.37

Predicted: 3.48